U.S. Department of Energy's
Office of Science

Software 'Effectiveness'

Advanced Scientific Computing Advisory Committee

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OMB Measure

- Improve Computational Science Capabilities. Average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the Scientific Discovery through Advanced Computing (SciDAC) effort. FY05 – >50%

FY 2003 Codes

- AGILE-BOLTZTRAN – time to solution for a baseline run of size 8x12x100 (8 angles, 12 energy groups, and a spatial resolution of 100).
- BEAMBEAM3D – total computational effort achievable in the simulation, represented by the product of the number of particle-turns, the number of collisions per turn, and the square of the number of longitudinal slices.
- AMR Combustion – the product of the number of chemical reactions simulated times the number of effective zones, a measure of the effective resolution achieved throughout the computational domain.
- NIMROD – the time required for simulation of the nonlinear tearing evolution over the transport timescale.

FY 2003 Results

- AGILE-BOLTZTRAN. Simulation time in 2002: 4 weeks. Simulation time in 2003: 4 days. Improvement in effectiveness: 700%
- BEAMBEAM3D. Maximum computational effort in 2002: 1011. Maximum computational effort in 2003: 1012. Improvement in effectiveness: 1,000%.
- AMR Combustion. Reactions x zones in 2002: 3.5x108. Reactions x zones in 2003: 3.7x1010. Improvement in effectiveness: 10,571%.
- NIMROD – Simulation time in 2002: 5.5 days. Simulation time in 2003: 2 days. Improvement in effectiveness: 275%

FY 2004 Proposed Codes

- Global Climate CCSM
- Shell Model Monte Carlo (SMMC)
- Virginia Hydrodynamics 1 (VH-1)
- The MILC Code (QCD)
- Parallel R-Matrix with Pseudostates

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CCSM

- The scientific objectives of the CCSM program are as follows:
  - Develop and continuously improve a comprehensive climate modeling system that is at the forefront of international efforts to understand and predict the behavior of Earth's climate.
  - Use this modeling system to investigate and understand the mechanisms that lead to interdecadal, interannual, and seasonal variability in Earth's climate.
  - Explore the history of Earth's climate through the application of versions of the CCSM suitable for paleoclimate simulations.
  - Apply this modeling system to estimate the likely future of Earth's environment in order to provide information required by governments in support of local, state, national, and international policy determination.
- DOE Contacts:
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SMMC

- The Shell Model Monte Carlo (SMMC) code will be used to investigate thermal properties of nuclei in the mass 80-120 region. Nuclei in this region, exhibit extremely interesting pairing and shape transitions as a function of increasing temperature. This nuclear region also plays an important role in the electron-capture and neutrino-nucleus scattering that occurs during the core collapse of type II supernovae. We will investigate these phenomena using quantum Monte Carlo algorithms adapted to the nuclear shell model. Our code currently runs on platforms at NERSC and ORNL and is naturally parallel. The per-processor speed of the code is 350 MFlops on Seaborg at NERSC, and scales naturally to as many processors as are needed for a particular application.
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VH-1

- Description of the Code: VH-1 is a three-dimensional, PPM hydrodynamics code capable of simulating three-dimensional turbulent stellar flows with high accuracy and little dissipation (in other words, it is able to track features very well over long simulations).

- Description of the Problem: Three-dimensional simulations of "accretion" disks around black holes. The spiraling inflow of material onto a central black hole is likely a key part of the central engine for a class of core collapse supernovae that are hyperenergetic ("hypernovae") and associated with gamma ray bursts. High-resolution, three-dimensional simulations to understand this inflow are critical in order to eventually understand this central engine and the associated supernova mechanism and gamma ray bursts.

- Contact:

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The MILC Code

- The MILC Code: This code, which is publicly available, has been in existence for over fifteen years. It is highly portable, and has run on virtually all computers available to members of the academic community during its lifetime. It is written in C. Compiler options allow the user to choose among MPI, a number of proprietary message passing packages, and the new QCD API message passing interface, QMP. Compiler options also allow the user to choose different formulations of QCD on the lattice, different algorithms for carrying out the simulations, and a wide variety of different physics applications. Since the start of the SciDAC Program, the performance of this code has been significantly enhance, and its applicability extended to the latest in the line of special purpose computers designed at Columbia University, the QCDOC.
- Contact person: Robert Sugar

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Parallel R-Matrix with Pseudostates

- Atomic, molecular, and particle-surface interactions are a key area of research supporting plasma sciences such as fusion energy, atmospheric research, and technical processing of semiconductors, as well as being of great fundamental interest. Newly developed computational methods implemented on US DOE parallel supercomputers through our participation in SciDAC have lead to dramatically revised rate coefficients for electron-impact processes of importance in plasma science utilizing the R-Matrix with Pseudostates (RMPS) code. RMPS is parallelized via use of SCALAPACK linear algebra routines and other means of distributing computation involved in solving the Schrodinger partial differential equation for electrons inelastically scattering from many-electron target atoms and ions.
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